

Alternating-Spin Ladders

Takahiro Fukui*

Institute of Advanced Energy, Kyoto University, Uji, Kyoto 611, Japan

Norio Kawakami

Department of Applied Physics, Osaka University, Suita, Osaka 565, Japan

(May 7, 1997; Revised, August 18, 1997)

We investigate a two-leg spin ladder system composed of alternating-spin chains with two-different kind of spins. The fixed point properties are discussed by using spin-wave analysis and non-linear sigma model techniques. The model contains various massive phases, reflecting the interplay between the bond-alternation and the spin-alternation.

PACS: 75.10.Jm, 05.30.-d, 03.65.Sq

I. INTRODUCTION

Since the seminal work of Haldane¹, quantum spin chains have been extensively studied as one of the simplest but the most typical quantum many-body systems. The fixed-point properties of such systems depend on whether the spin is integer or half-integer, as shown by the use of the non-linear sigma model (NLSM) with a topological term^{1,2}. The massive phase of the integer-spin chains, called Haldane phase, has been understood as valence-bond-solid (VBS) states proposed by Affleck et al.³. Quantum phase transitions caused by the bond-alternation have been predicted⁴ and have been confirmed numerically⁵, which in fact fits in with the VBS picture. Current interest has been spread to wider classes of spin chains, stimulated by experimental realization of a variety of spin systems. A typical example is the spin ladder system⁶⁻⁸, owing to the discovery of the high-temperature superconductivity, and another is the alternating-spin chain composed of two kind of spins⁹⁻¹¹.

In this paper, we propose and investigate a novel spin model, stimulated by recent interests mentioned-above, i.e., a two-leg spin ladder model composed of alternating-spin chains with some kind of bond-alternations. This type of spin systems are expected to be synthesized experimentally in future, and thus could provide an interesting example in quantum spin systems. What is particularly interesting in this model is that *one can explicitly see the interplay between the bond-alternation and the spin-alternation, both of which affect the quantum phase transitions*. We first study the model by the spin-wave analysis, and then by mapping it to the NLSM we demonstrate that it is not only the bond-alternation but also the spin-alternation which gives rise to a rich structure for the phase diagram.

II. THE MODEL

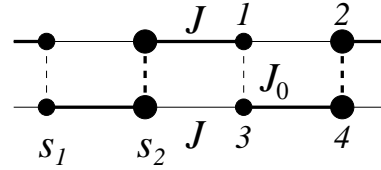


FIG. 1. Schematic illustration of the model.

The model we investigate (see Fig.1) is a two-leg spin ladder system composed of alternating-spin chains with two kind of spins s_1 and s_2 , defined by

$$H = \sum_{j=1}^N \left[\sum_{i=1}^2 J \Gamma_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} + J_0 \Gamma_{0,j} \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j} \right], \quad (1)$$

where $\Gamma_{i,j}$ are bond-alternation parameters

$$\Gamma_{i,j} = \begin{cases} 1 - \gamma_i & \text{for } j = \text{odd} \\ 1 + \gamma_i & \text{for } j = \text{even} \end{cases}, \quad (2)$$

for $i = 0, 1, 2$, and N ($= \text{even}$) is the number of sites for each chain. We denote the spin of the j th site of the i th chain as $s_{i,j}$, where

$$s_{i,j} = \begin{cases} s_1 & \text{for } j = \text{odd} \\ s_2 & \text{for } j = \text{even} \end{cases}, \quad (3)$$

for $i = 1, 2$. What is interesting is that the model naturally interpolates two kind of alternating-spin chains. Namely, when $J_0 = 0$ it reduces to two independent alternating-spin chains $s_1 \otimes s_2 \otimes s_1 \otimes s_2 \otimes \dots$ with ferrimagnetic ground state¹⁰. On the other hand, when $\gamma_1 = 1$ and $\gamma_2 = -1$ ($J_0 \neq 0$) it becomes a single “alternating-spin chain” $s_1 \otimes s_1 \otimes s_2 \otimes s_2 \otimes \dots$ with a singlet ground state, which has recently been studied in ref.¹²⁻¹⁴. In what follows, we restrict ourselves to antiferromagnetic couplings $0 < J$, $0 < J_0$ and $-1 < \gamma_i < 1$. Then the ground state proves to be a unique singlet.

III. SPIN-WAVE MODES

Analysis of the spin-waves is indispensable to mapping to the NLSM, since the mapping is ensured by the

linear-dispersion relation of the spin-wave mode above the classical Néel ground state. For this purpose, it is suitable to introduce four kind of bosons to express the spin generators by the use of the Holstein-Primakoff mapping (see Fig.1 for the numbering), assuming the Néel configuration. In the momentum space, the spin-wave Hamiltonian of quadratic order in boson operators is calculated as $H_{\text{sw}} = \sum_{k=1}^{N/2} \mathbf{A}^\dagger \mathcal{H} \mathbf{A}$, where $\mathcal{H} = \begin{pmatrix} h & \Delta \\ \bar{\Delta} & \bar{h} \end{pmatrix}$. In this equation, we have defined $A_i = a_i$ (a_i^\dagger) for $i = 1 \sim 4$ ($5 \sim 8$) and 4×4 matrices h and Δ

$$h = J \text{diag}(s_2, s_1, s_2, s_1) + \frac{J_0}{2} \text{diag}(\Gamma_- s_1, \Gamma_+ s_2, \Gamma_- s_1, \Gamma_+ s_2),$$

$$\Delta = \frac{1}{2} \begin{pmatrix} 0 & \Delta_1 & \Delta_- & 0 \\ \Delta_1 & 0 & 0 & \Delta_+ \\ \Delta_- & 0 & 0 & \Delta_2 \\ 0 & \Delta_+ & \Delta_2 & 0 \end{pmatrix}, \quad (4)$$

where

$$\begin{aligned} \Delta_j &= 2J\sqrt{s_1 s_2} (\cos p + (-)^j i \gamma_j \sin p), \\ \Delta_+ &= J_0 \Gamma_+ s_2, \\ \Delta_- &= J_0 \Gamma_- s_1. \end{aligned} \quad (5)$$

We have denoted the momentum as $p \equiv 2\pi k/N$ with integers $k = 1, \dots, N/2$. Here and in what follows, we occasionally use a simpler notation $\Gamma_\pm \equiv 1 \pm \gamma_0$. Now introduce the Bogoliubov transformation $\mathbf{A} = \mathcal{U} \mathbf{B}$, where \mathcal{U} is a 8×8 matrix. If the transformed operators \mathbf{B} satisfy the boson commutation relations, the matrix \mathcal{U} should satisfy $\mathcal{U} \mathcal{N} \mathcal{U}^\dagger = \mathcal{U}^\dagger \mathcal{N} \mathcal{U} = \mathcal{N}$, where we have introduced the metric $\mathcal{N} = \text{diag}(1_4, -1_4)$ with 1_4 being the 4×4 unit matrix.

The spin-waves are composed of four modes in general. However, in the case $\gamma_1 = -\gamma_2$ two of them become degenerate and we have only two modes. In what follows, we restrict ourselves to this simple case, and investigate especially the effects of γ_0 and its interplay with the spin-alternation for the ground state properties of the model. For this purpose, we will simplify the notations,

$$\gamma_1 = -\gamma_2 \equiv \gamma_\parallel, \quad \gamma_0 \equiv \gamma. \quad (6)$$

For this simple case, we can diagonalize the spin-wave Hamiltonian and explicitly obtain the dispersion relations of the form

$$\omega_\pm = \sqrt{2} \sqrt{A \sin^2 p + B \pm \sqrt{(2AB - C) \sin^2 p + B^2}}, \quad (7)$$

where

$$\begin{aligned} A &= 2J^2(1 - \gamma_\parallel^2) s_1 s_2 \\ B &= J[J(s_1 - s_2)^2 + 2J_0 s_1 s_2] \\ C &= 4J^2 J_0 s_1 s_2 \{ J(1 - \gamma_\parallel^2) [(1 - \gamma) s_1^2 + (1 + \gamma) s_2^2] \\ &\quad + J_0(1 - \gamma^2) s_1 s_2 \} \end{aligned} \quad (8)$$

The lower spin-wave mode in eq.(7) is thus found to have a linear dispersion for small momenta, $\omega_- \sim v_s p$, where

$$v_s = \sqrt{C/B}. \quad (9)$$

In Fig.2, we present some examples of these modes.

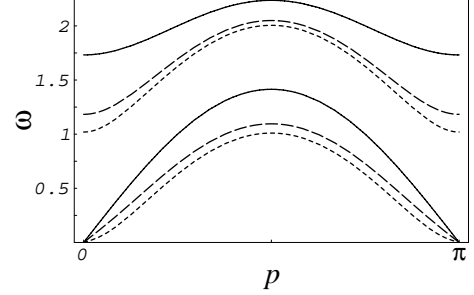


FIG. 2. Spin-wave spectrum as functions of the momentum p for $J_0 = 0.01$ (dotted line) 0.1 (dashed line) and 0.5 (solid line) with other parameters being fixed as $s_1 = 1/2$, $s_2 = 1$, $J = 1$ and $\gamma_0 = \gamma_1 = \gamma_2 = 0$.

First, let us look at the dotted line in Fig.2, which is calculated for rather small inter-chain coupling $J_0 = J/100$. Note that it resembles, in this energy scale, the quadratic dispersion relation for the ferrimagnetic case, $\omega_\pm/J = \pm|s_2 - s_1| + [(s_1 - s_2)^2 + 4s_1 s_2 \sin^2 p]^{1/2}$. However, from eq.(7), the lower mode is always linear as far as $J_0 \neq 0$, even though its linearity is restricted to small momentum region. This reflects the fact that the ground state is always singlet in spite of the magnitude of $J_0 (\neq 0)$. In fact, if we increase the inter-chain coupling J_0 up to $\sim J/10$ (dashed-line), we can explicitly see that the lower mode has a linear dispersion in a wider momentum region. Therefore, even for rather small J_0 , we expect that the model can be described by the NLSM at least qualitatively.

IV. O(3) NONLINEAR SIGMA MODEL APPROACH

We have so far investigated the classical properties of the ground state. However, the low-energy quantum fluctuation plays an essential role in determining the true ground state. In order to investigate them, we will use NLSM techniques^{1,2,15-17}. Introducing the SU(2) coherent state by $\langle \mathbf{n}_{i,j} | \mathbf{S}_{i,j} | \mathbf{n}_{i,j} \rangle = s_{i,j} (-)^{i+j} \mathbf{n}_{i,j}$, we have the effective action given by $S = S_B + S_I$, where

$$\begin{aligned} S_B &= -i \sum_{i=1}^2 \sum_{j=1}^N s_{i,j} (-)^{i+j} \omega[\mathbf{n}_{i,j}], \\ S_I &= - \sum_{j=1}^N \left(\sum_{i=1}^2 J \Gamma_{i,j} \int_0^\beta d\tau \mathbf{n}_{i,j} \cdot \mathbf{n}_{i,j+1} \right. \\ &\quad \left. + J_0 \Gamma_{0,j} \int_0^\beta d\tau \mathbf{n}_{1,j} \cdot \mathbf{n}_{2,j} \right), \end{aligned} \quad (10)$$

Here, $\omega[\mathbf{n}]$ is the Berry phase defined by $\omega[\mathbf{n}] = \int_0^\beta d\tau \int_0^1 d\mathbf{u} \cdot (\partial_\tau \mathbf{n} \times \partial_u \mathbf{n})$.

Now introduce the semi-classical Néel configuration \mathbf{m} and fluctuations \mathbf{l}_a around it as follows,

$$\mathbf{n}_{i,2j+a} = \mathbf{m}(2j+a) + (-)^{i+a} a_0 \mathbf{l}_a(2j+a), \quad (11)$$

for $i = 1, 2$, $j = 0, 1, \dots, N/2 - 1$ and for $a = 1, 2$, where a_0 is a lattice constant. We have introduced two kind of the fluctuation fields \mathbf{l}_1 and \mathbf{l}_2 ¹⁵⁻¹⁷, by taking into account the fact that we have two spin-wave modes in the above spin-wave analysis. Now the calculation is straightforward, and we reach the lagrangian

$$\mathcal{L} = \frac{1}{2} \mathbf{l}_a L_{ab} \mathbf{l}_b + i u_a \mathbf{l}_a \cdot (\mathbf{m} \times \partial_\tau \mathbf{m}) + v_a \mathbf{l}_a \cdot \partial_x \mathbf{m} + w (\partial_x \mathbf{m})^2 \quad (12)$$

where repeated indices a and b should be summed over, and where

$$L = 2 \begin{pmatrix} J s_1 s_2 + J_0 \Gamma_- s_1^2 & J s_1 s_2 \\ J s_1 s_2 & J s_1 s_2 + J_0 \Gamma_+ s_2^2 \end{pmatrix}, \quad \mathbf{u}^t = (s_1, s_2), \quad \mathbf{v}^t = 2J\gamma_{\parallel} s_1 s_2 (1, 1), \quad w = J s_1 s_2. \quad (13)$$

Here, the couplings J and J_0 mean those in unit of a_0 .

Integrating out the fields \mathbf{l} , we end up with

$$\mathcal{L} = \frac{1}{2g} \left[v_s (\partial_1 \mathbf{m})^2 + \frac{1}{v_s} (\partial_2 \mathbf{m})^2 \right] + \frac{\theta}{8\pi} \epsilon_{\mu\nu} \mathbf{m} \cdot (\partial_\mu \mathbf{m} \times \partial_\nu \mathbf{m}), \quad (14)$$

where

$$\begin{aligned} \theta &= 4\pi i \mathbf{u}^t L^{-1} \mathbf{v} \\ &= \frac{4\pi i \gamma_{\parallel} s_1 s_2 [(1-\gamma)s_1 + (1+\gamma)s_2]}{(1-\gamma)s_1^2 + (1+\gamma)s_2^2 + R(1-\gamma^2)s_1 s_2}, \\ g &= [(2w - \mathbf{v}^t L^{-1} \mathbf{v}) \mathbf{u}^t L^{-1} \mathbf{u}]^{-1/2}, \\ v_s &= [(2w - \mathbf{v}^t L^{-1} \mathbf{v}) / \mathbf{u}^t L^{-1} \mathbf{u}]^{1/2}. \end{aligned} \quad (15)$$

Here we have defined the ratio $R = J_0/J$. What is remarkable is that the spin-wave velocity calculated here coincides exactly with eq.(9), which implies that the present NLSM approach is consistent with the spin-wave analysis. Before discussing the phase diagram, we will check the formulae (15) by comparing them with those in some limits we have already known. First, set $s_1 = s_2 \equiv s$ and $\gamma = 0$, and we have $\theta/\pi i = 8s\gamma_{\parallel}/(2+R)$, exactly coinciding with the formula in ref.¹⁶ for the usual two-leg ladder with intra-chain bond-alternation. Set furthermore $\gamma_{\parallel} = 0$, we have $\theta = 0$, $g = 1/s \times (1+R/2)^{1/2}$ and $v_s = 2sJ(1+R/2)^{1/2}$, which correctly reproduce the formulae in^{15,17} for the usual uniform ladder. Next, set $\gamma_{\parallel} = 1$, $\gamma = 0$, $J = J'(1+\gamma')/2$, and $J_0 = J'(1-\gamma')$, then we have the expression $\theta = 4\pi i(1+\gamma')s_1 s_2 (s_1 + s_2)/[(s_1 + s_2)^2 + \gamma'(s_1 - s_2)^2]$, etc, derived in¹⁴ for the single $s_1 \otimes s_1 \otimes s_2 \otimes s_2 \otimes \dots$ chain.¹⁸

V. PHASE DIAGRAM

Now let us investigate various phases of the model. First of all, the formula (15) tells us that if $\gamma_{\parallel} = 0$ we have always $\theta = 0$, leading to massive phases. In other words, *non-trivial massless phases can occur if $\gamma_{\parallel} \neq 0$* . In what follows, we assume $\gamma_{\parallel} \neq 0$ and investigate the phases of the model. Let us first consider the case $s_2 \rightarrow \infty$, for example. We have $\theta \rightarrow 4\pi i \gamma_{\parallel} s_1$, i.e, the phases of the model are controlled only by the smaller spin, independent of R and γ . This simple statement is, needless to say, valid only for this case: In the rest of the paper, we investigate the properties of the phase transitions in more general cases, putting stress on how the spin-alternation affects them. In what follows, we set $s_1 \leq s_2$ for simplicity. As the intra-chain bond-alternation γ_{\parallel} has been already discussed in ref.¹⁶, we concentrate on the inter-chain bond-alternation γ ($= \gamma_0$) and its interplay with the spin-alternation, assuming $0 \leq \gamma_{\parallel}$ without loss of generality. Setting $\theta/(\pi i) \equiv n$ with n being an odd integer, we can draw in the R - γ plane the critical lines on which the model is expected to be massless,

$$R = \frac{s_1}{1+\gamma} \left(\frac{4\gamma_{\parallel}}{n} - \frac{1}{s_2} \right) + \frac{s_2}{1-\gamma} \left(\frac{4\gamma_{\parallel}}{n} - \frac{1}{s_1} \right). \quad (16)$$

We can see that according to the value of n there appear three kind of lines (see Fig.3),

- (i) $n < 4\gamma_{\parallel} s_1$,
- (ii) $n = 4\gamma_{\parallel} s_1$,
- (iii) $4\gamma_{\parallel} s_1 < n < 4\gamma_{\parallel} s_2$.

The line (ii) exists only the case in which $4\gamma_{\parallel} s_1$ happens to be an odd integer. The lines (ii) and (iii) can exist only if the two kind of the spins are different, $s_1 \neq s_2$. In other words, *the effects of the spin-alternation can be observed typically by the existence of lines of the types (ii) and (iii)*.

We note that in the region near the γ axis (with quite small R), the present approximation may become worse, because when exactly $R = 0$, the model decouples to two independent alternating-spin chains with ferrimagnetic ground state, which cannot be described by the present approach. However, as noted above, as long as $J_0 \neq 0$ we always have a linear spin-wave dispersion even though it is restricted, for small J_0 , in a small momentum region. Therefore, we believe that the phase diagram in the R - γ plane is qualitatively valid even for small R .

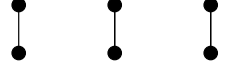
A. $s_1 = s_2$ case

Because the inter-chain bond-alternation is introduced, as far as we know, for the first time in this paper, let us first consider the usual ladder system with $s_1 = s_2$. What we would like to claim here is that the inter-chain

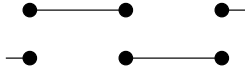
bond-alternation really affects θ once the finite intra-chain bond-alternation is introduced even for the usual $s_1 = s_2 = 1/2$ ladder as follows:

- (1) for $1/2 < \gamma_{\parallel} < 1$ we have only one massless line $R = 2(2\gamma_{\parallel} - 1)/(1 - \gamma^2) \equiv R_1(\gamma)$, corresponding to $n = 1$,
- (2) for $0 \leq \gamma_{\parallel} \leq 1/2$ we have no massless line.

In case (1), we expect to have the VBS state



in the region $R > R_1(\gamma)$ while in the opposite region $R < R_1(\gamma)$ we may have the state



between which we have a massless phase. Contrary to this, in case (2), we have the former VBS state in the whole R - γ plane. From these observations, we see that the inter-chain bond-alternation indeed affects the phase structure.

B. $s_1 \neq s_2$ case

Now let us discuss the model with $s_1 = 1/2$ and $s_2 = 1$, which may be one of the most probable candidates for the experimental observation of the alternating-spin ladders. The phase diagram is qualitatively classified into

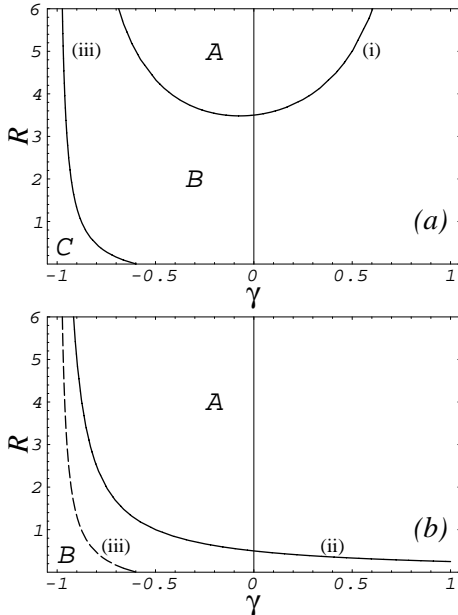


FIG. 3. The phase diagram for $s_1 = 1/2$ and $s_2 = 1$. (a): $\gamma_{\parallel} = 1$. (b): $\gamma_{\parallel} = 1/2$ for solid line and $\gamma_{\parallel} = 1/3$ for dashed line.

(I) $3/4 < \gamma_{\parallel} \leq 1$, (II) $1/2 < \gamma_{\parallel} \leq 3/4$, (III) $\gamma_{\parallel} = 1/2$, (IV) $1/4 < \gamma_{\parallel} < 1/2$ and (V) $\gamma_{\parallel} \leq 1/4$, according to

how many critical lines of the categories (i), (ii) and (iii) appear. In Fig.3, we present some examples of the phase diagram. In Fig.3(a), there appear three kind of massive phases separated by two massless lines (case (I)). If we trace the phase diagram along the R -axis ($\gamma = 0$ line), we can easily specify the phases A and B in terms of

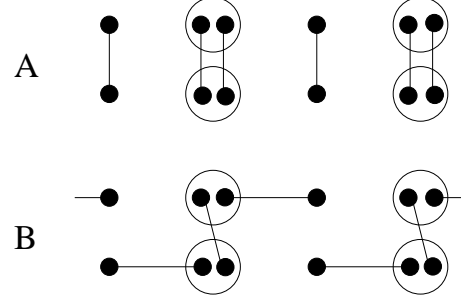


FIG. 4. VBS states for the phases A and B.

VBS picture in Fig.4 (in the case $\gamma_{\parallel} = 1$ see¹²). What is most interesting is the appearance of the new phase C, separated from the others by another massless line which belongs to the category (iii). Namely this phase is caused by the interplay between the bond-alternation and the spin-alternation. In order to see what kind of the ground state is indeed realized in the phase C, let us first start with a point in the region A, and move parallel to γ -axis toward the $\gamma = -1$ direction. In this process, the interaction between two $s_2 = 1$ spins is decreased, so that one of the valence-bond changes its partner, and we thus reach the phase B. Then the question is what happens when the interaction between two $s_1 = 1/2$ spins is further increased. We then expect that $s_1 = 1/2$ spins form the valence-bond, and as a consequence $s_2 = 1$ spins cannot help forming the valence-bond again, which results in the phase C. Therefore, it is natural to conclude that the resulting ground state in the phase C is identical to that in the phase A. So far we have discussed the phase diagram of (I). The diagram of (II) is similar to (I), but without the line (iii) in Fig.3(a) and hence without the phase C.

Shown in Fig.3(b) is another example of the phase diagram for which the critical line is essentially determined by the spin-alternation itself (cases (III) and (IV)). What is to be noted is the difference between two cases, the critical line for which is indicated by the solid line ($\gamma_{\parallel} = 1/2$) and the dashed line ($\gamma_{\parallel} = 1/3$). For example, if we change the ratio of R with $\gamma = 0$ being fixed, we encounter the phase transition in the former case, while in the latter case we are always in the A phase. Also, if we start from $\gamma = -1$ with rather small R towards $\gamma = 1$ direction, we may be always in the phase B in the former case, while in the latter case we experience the transition from the phase B to A before $\gamma = 0$. We note that the phase diagram of (V) has no critical lines, and hence has

only the phase A.

VI. SUMMARY AND DISCUSSIONS

We have proposed a spin-alternating ladder model, which shows interesting interplay between the bond-alternation and the spin-alternation. We have indeed shown how the spin-alternation affects the quantum phase transitions, and have derived the phase diagram by means of $O(3)$ nonlinear sigma model techniques.

Here, some comments are in order. First we wish to mention the effects of frustration which have been ignored in this paper. For example, if we include the next-nearest interaction, some interesting phenomena may be expected to happen. However, as far as such frustration is small enough to be treated as a perturbation, it merely renormalizes the coupling g and the velocity v_s , for which the present conclusion may be still valid. The detailed study on the effect of frustration is an interesting issue to be explored in the future study. Another comment is on the quantitative arguments for the phase diagram. Even for ordinary spin chains, the predicted values by the NLSM for the bond-alternation parameter which causes massless phases⁴ are slightly different from those obtained by numerical calculations⁵. Nevertheless, it is believed that the NLSM can describe qualitatively correct low-energy properties, and the number of the massless phases in varying the bond-alternation parameter is correctly predicted. We believe that these statements are also the case for our model, and the present analysis based on the NLSM should provide the qualitatively correct phase diagram, although the predicted critical lines should be somehow modified by more accurate treatment.

To conclude the paper, we wish to emphasize again that although the model we proposed in this paper seems somewhat complicated at first sight, it is a generalized model which naturally interpolates various interesting quantum spin systems investigated intensively. For example, if we set $\gamma = 1$, the model is reduced to a single chain composed of two kind of spins, while for the case $\gamma = 0$ and $s_1 = s_2$ it becomes a usual ladder model. What is the merit of studying the present model is that a wider class of spin models can be treated on an equal footing. So far, spin ladder systems with the spin-alternation have not been found experimentally. We hope that a ladder system proposed here, or a system which naturally interpolates spin chains and ladders can be realized experimentally in the near future. These issues then provide new paradigms of the quantum phase transitions for low-dimensional spin systems. In such cases, the present model could serve as a key model which connects the physics of various spin systems such as the spin ladder, the alternating spin chain, etc.

ACKNOWLEDGMENTS

The authors would like to thank T. Tonegawa, M. Kaburagi and M. Chiba for valuable discussions. This work is partly supported by the Grant-in-Aid from the Ministry of Education, Science and Culture, Japan.

* Email: fukui@yukawa.kyoto-u.ac.jp

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¹⁸ Note that the present formula for v_s is half as large as that in¹⁴, because of the difference of the definition of the momentum. In the snake chain ($\gamma_{\parallel} = 1$), the length of the system is twice as long as the usual single chain.